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I U C L I D

Data Set

Existing Chemical : ID: 117-84-0
CAS No. : 117-84-0
EINECS Name : dioctyl phthalate
EC No. : 204-214-7
TSCA Name : 1,2-Benzenedicarboxylic acid, dioctyl ester
Molecular Formula : C₂₄H₃₈O₄

Producer related part
Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 18.10.2000

Substance related part
Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 18.10.2000

Status :
Memo : ACC Phthalate Ester Panel HPV Testing Group

Printing date : 07.12.2006
Revision date :
Date of last update : 07.12.2006

Number of pages : 26

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 117-84-0
Date 07.12.2006

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : lead organisation
Name : ACC Phthalate Esters Panel HPV Testing Group
Contact person : Dr. Marian Stanley
Date :
Street : 1300 Wilson Blvd.
Town : 22209 Arlington, VA
Country : United States
Phone : (703) 741-5623
Telefax : (703) 741-6091
Telex :
Cedex :
Email :
Homepage :

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes eleven CAS numbers (see the Freertext Remark section for complete list).

Remark : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following eleven CAS numbers:
68648-93-1 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)
117-84-0 1,2-benzenedicarboxylic acid, dioctyl ester (DOP)
16883-83-3 1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)
68515-40-2 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl (B79P)
68515-45-7 1,2-benzenedicarboxylic acid, dinonyl ester, branched and

linear (DNP)

68515-43-5 1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters (911P)

84-77-5 1,2-benzenedicarboxylic acid, didecyl ester (DDP)

3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (DUP)

85507-79-5 1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)

111381-91-0 1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)

68515-47-9 1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250°C) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

08.05.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :

1. General Information

Id 117-84-0
Date 07.12.2006

Substance type : organic
Physical status : liquid
Purity :
Colour :
Odour :

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Polymers industry

Remark : High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

Id 117-84-0
Date 07.12.2006

2.1 MELTING POINT

Value : -25 °C
Decomposition : no, at °C
Sublimation :
Method : other: no data
Year :
GLP :
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Remark : Data are from a peer reviewed literature review of data from a variety of sources including manufacturer's data or handbook values.

Test substance : CAS #117-84-0; dioctyl phthalate
Reliability : (2) valid with restrictions
This robust summary is assigned a reliability of 2 because there is limited information on how the data were developed.

Flag : Critical study for SIDS endpoint
06.07.2006 (9)

Value : 90 °C
Decomposition : no, at °C
Sublimation : no
Method : other: calculation
Year :
GLP :
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Method : Melting point calculation by MPBPWIN ver. 1.41 using calculation methods of Joback and Gold and Ogle.

Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation. However, the melting point calculation in EPI Suite™ gives erroneously high results for the phthalate esters.

Test substance : CAS #117-84-0; dioctyl phthalate
Reliability : (3) invalid
02.06.2006 (4)

2.2 BOILING POINT

Value : 431 °C at 1013 hPa
Decomposition : no
Method : other
Year :
GLP :
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Method : Boiling point calculation by MPBPWIN ver. 1.41 using calculation method of Stein and Brown.

Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation.

Test substance : CAS #117-84-0; dioctyl phthalate
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
02.06.2006 (4)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .000000133 hPa at 25 °C
 Decomposition : no
 Method : other (calculated)
 Year :
 GLP :
 Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Method : Measured data collected and tabulated, calculated data also considered in determining recommended values.

Remark : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for vapour pressure, represent the definitive and currently accepted physicochemical database for selected phthalate esters including dioctyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm³ mol⁻¹). The Le Bas molar volume used for dioctyl phthalate ester was 520.4 cm³ mol⁻¹.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
 r² = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
 r² = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
 r² = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : CAS #117-84-0; dioctyl phthalate
 Reliability : (2) valid with restrictions

The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
 02.06.2006

(1)

Value : .000001933 hPa at 25 °C
 Decomposition : no
 Method : other (calculated)
 Year :
 GLP :
 Test substance : other TS: CAS #117-84-0; dioctyl phthalate

2. Physico-Chemical Data

Id 117-84-0

Date 07.12.2006

Method : Vapor pressure calculation by MPBPWIN ver. 1.41 using calculation method of Grain.
Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS #117-84-0; dioctyl phthalate
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

02.06.2006

(4)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : 7.73 at 25 °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Method : Measured data collected and tabulated, calculated data also considered in determining recommended values.

Remark : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for partition coefficient, represent the definitive and currently accepted physicochemical database for selected phthalate esters including dioctyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume ($\text{cm}^3 \text{mol}^{-1}$). The Le Bas molar volume used for dioctyl phthalate ester was $520.4 \text{ cm}^3 \text{mol}^{-1}$.

$\text{Log CS(WL)} = -0.012V + 5.8$, $n = 35$ (solubility in water)
 $r^2 = 0.98$, $\text{SE} = 0.39$

$\text{Log CS(AL)} = -0.013V - 1.3$, $n = 15$ (solubility in air)
 $r^2 = 0.87$, $\text{SE} = 0.33$

$\text{Log CS(OL)} = -0.016V + 3.4$, $n = 68$ (solubility in octanol)
 $r^2 = 0.19$, $\text{SE} = 0.41$

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : CAS #117-84-0; dioctyl phthalate
Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint

02.06.2006

(1)

Partition coefficient : octanol-water
Log pow : 8.54 at 25 °C
pH value :

2. Physico-Chemical Data

Id 117-84-0

Date 07.12.2006

Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Method : Partition coefficient by LOGKOWWIN ver. 1.67 using an atom/fragment calculation method of Meylan and Howard.
Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS #117-84-0; dioctyl phthalate
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

02.06.2006

(4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : .00249 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Method : Measured data collected and tabulated, calculated data also considered in determining recommended values.

Remark : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for water solubility, represent the definitive and currently accepted physicochemical database for selected phthalate esters including dioctyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume ($\text{cm}^3 \text{mol}^{-1}$). The Le Bas molar volume used for dioctyl phthalate ester was $520.4 \text{ cm}^3 \text{mol}^{-1}$.

$\text{Log CS(WL)} = -0.012V + 5.8$, $n = 35$ (solubility in water)
 $r^2 = 0.98$, $\text{SE} = 0.39$

$\text{Log CS(AL)} = -0.013V - 1.3$, $n = 15$ (solubility in air)
 $r^2 = 0.87$, $\text{SE} = 0.33$

$\text{Log CS(OL)} = -0.016V + 3.4$, $n = 68$ (solubility in octanol)
 $r^2 = 0.19$, $\text{SE} = 0.41$

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths

2. Physico-Chemical Data

Id 117-84-0
Date 07.12.2006

Test substance : from 1 to 13 carbons.
Reliability : CAS #117-84-0; dioctyl phthalate
: (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
02.06.2006 (1)

Solubility in : Water
Value : .00018 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Method : Water solubility calculated using WSKOWN ver 1.41 based on Kow correlation method of Meylan and Howard. Kow used in calculation was 8.54.

Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation.

Test substance : CAS #117-84-0; dioctyl phthalate
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

02.06.2006 (4)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2. Physico-Chemical Data

Id 117-84-0
Date 07.12.2006

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	: air
Light source	: Sun light
Light spectrum	: nm
Relative intensity	: 1 based on intensity of sunlight
Conc. of substance	: at 25 °C
INDIRECT PHOTOLYSIS	
Sensitizer	: OH
Conc. of sensitizer	: 1500000 molecule/cm ³
Rate constant	: .0000000002058 cm ³ /(molecule*sec)
Degradation	: 50 % after 6.2 hour(s)
Deg. product	: not measured
Method	: other (calculated)
Year	:
GLP	:
Test substance	: other TS: CAS #117-84-0; dioctyl phthalate
Method	: Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson.
Remark	: 50% degradation after 6.24 hrs or 0.52 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration. EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	: CAS #117-84-0; dioctyl phthalate
Reliability	: (2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	: Critical study for SIDS endpoint
02.06.2006	(4)

3.1.2 STABILITY IN WATER

Type	: abiotic
t1/2 pH4	: at °C
t1/2 pH7	: 7.7 year at 25 °C
t1/2 pH9	: at °C
Deg. product	: not measured
Method	: other (calculated)
Year	:
GLP	:
Test substance	: other TS: CAS #117-84-0; dioctyl phthalate
Method	: Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	: EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	: CAS #117-84-0; dioctyl phthalate
Reliability	: (2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	: Critical study for SIDS endpoint

3. Environmental Fate and Pathways

Id 117-84-0
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3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
-----------	----------------

Molecular Weight	390.57
Temperature	25° C
Log Kow	7.73
Water Solubility	0.00249 g/m3
Vapor Pressure	0.0000133 Pa
Melting Point	-25°C

Result : Using the Mackay Level I calculation, the following distribution is predicted for dioctyl phthalate:

% Distribution	Compartment
0.0	Air
0.1	Water
97.8	Soil
2.2	Sediment
0.1	Suspended Sediment
0.0	Biota

Test substance : CAS #117-84-0; dioctyl phthalate
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint

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(7)

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
-----------	----------------

Molecular Weight	390.57
Temperature	25° C
Log Kow	7.73

3. Environmental Fate and Pathways

Id 117-84-0
Date 07.12.2006

Water Solubility 0.00249 g/m3
Vapor Pressure 0.0000133 Pa
Melting Point -25°C

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
Air	12.48a
Water	120b
Soil	420c
Sediment	420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI Suite™ version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI Suite™, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from: Exxon Biomedical Sciences, Inc. (1995) and Boethling (2000):
Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Result

: Using the Mackay Level III calculation, the following distribution is predicted for dioctyl phthalate:

Compartment	% Distribution
Air	1.0
Water	8.3
Soil	68.7
Sediment	22.0

Test substance Reliability

: CAS #117-84-0; dioctyl phthalate
: (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag
02.06.2006

: Critical study for SIDS endpoint

(7)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3. Environmental Fate and Pathways

Id 117-84-0
Date 07.12.2006

3.5 BIODEGRADATION

Type : aerobic
Inoculum : other: River water
Concentration : .003 mg/l related to Test substance
related to
Contact time : 10 day(s)
Degradation : ca. 90 (±) % after 10 day(s)
Result :
Deg. product :
Method : other: River die away
Year :
GLP : no
Test substance : other TS: CAS #117-84-0; dioctyl phthalate; >=98% purity

Result : Dioctyl phthalate ester exhibited approximately 90% primary biodegradation in centrifuged Rhine River water samples after 10 days incubation at 20C. Samples incubated at 4C showed no biodegradative loss over the same time period.

Test condition : Water taken from the Rhine River in the vicinity of Lobith, The Netherlands, was used to assess the biodegradability of select phthalate esters including dioctyl phthalate ester at a low loading rate, 3 ppb, which is considered an environmentally relevant concentration. 500 ml of centrifuged river water was spiked with with phthalate ester. Two sets of samples were prepared and stored in the dark at two temperatures, 4 and 20C. Phthalate analysis was conducted by means of GC-MSD on days 0, 1, 3, 7, and 10. Recovery analyses resulted in recoveries of spiked samples, 0.1 mg/L, ranging from 82 to 83%. Phthalate was extracted from water samples by means of liquid-liquid extraction.

Test substance : CAS #117-84-0; dioctyl phthalate
Conclusion : The test substance is rapidly biodegradable.
Reliability : (2) valid with restrictions
This summary is rated a "2" and represents a key study, but does not follow a standard test procedure.

Flag : Critical study for SIDS endpoint
06.07.2006 (8)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

- 4.1 ACUTE/PROLONGED TOXICITY TO FISH
- 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES
- 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE
- 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA
- 4.5.1 CHRONIC TOXICITY TO FISH
- 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES
- 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS
- 4.6.2 TOXICITY TO TERRESTRIAL PLANTS
- 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS
- 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES
- 4.7 BIOLOGICAL EFFECTS MONITORING
- 4.8 BIOTRANSFORMATION AND KINETICS
- 4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : = 53700 mg/kg bw
Species : rat
Strain :
Sex : male
Number of animals :
Vehicle : no data
Doses :
Method : other
Year : 1987
GLP : no data
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Test condition : Rangefinding study used to establish dose levels for subsequent 5-day study. Only LD50 value reported; no information on animal numbers, dose levels, etc. provided.

Test substance : 1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate); CAS #117-84-0

Conclusion : Under the conditions of this study, the test substance has a low order of acute oral toxicity in rats.

Reliability : (2) valid with restrictions
There is insufficient information to rate the reliability of the data greater than 2. Although there was no information on animal numbers and dose levels, the study was peer reviewed and published.

07.12.2006

(2)

Type : LD50
Value : = 13000 mg/kg bw
Species : mouse
Strain :
Sex : male
Number of animals :
Vehicle : no data
Doses :
Method : other
Year : 1989
GLP : no data
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Test condition : Rangefinding study used to establish dose levels for subsequent 5-day study. Only LD50 value reported; no information on animal numbers, dose levels, etc. provided.

Test substance : 1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate); CAS #117-84-0

Conclusion : Under the conditions of this study, the test substance has a low order of acute oral toxicity in mice.

Reliability : (2) valid with restrictions
There is insufficient information to rate the reliability of the data greater than 2. Although there was no information on animal numbers and dose levels, the study was peer reviewed and published.

07.12.2006

(3)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	Daily
Frequency of treatm.	:	Daily for 13 weeks
Post exposure period	:	Not applicable
Doses	:	0, 5, 50, 500, or 5000 parts per million (0, 0.4, 3.8, 38.8, or 376.5 mg/kg/day).
Control group	:	yes
NOAEL	:	= 38.8 mg/kg
Method	:	OECD Guide-line 408 "Subchronic Oral Toxicity - Rodent: 90-day Study"
Year	:	1997
GLP	:	no data
Test substance	:	other TS: CAS #117-84-0; dioctyl phthalate
Method	:	One-way analysis of variance and Duncan's multiple range test.
Remark	:	No clinical signs of toxicity, reductions in body weight or food consumption were observed throughout the study. At the highest dose, DNOP caused threefold (females) and 12-fold (males) increases in liver ethoxyresorufin-O-deethylase activity while DEHP did not. Both DEHP and DNOP at 5000 ppm caused mild histological changes in the thyroid consisting of reduced follicle size and colloid density, and the liver consisting of endothelial nuclear prominence, nuclear hyperchromicity and anisokaryosis. There was accentuation of zonation of the hepatic lobules and increased perivenous cytoplasmic vacuolation in DNOP-treated rats. DNOP did not induce any testicular changes or visible increases in the number of peroxisomes. Trace quantities (3-5 ppm) of DEHP and DNOP were detected in the liver, and 15-31 ppm were found in adipose tissue of the highest dose groups.
Test condition	:	Sprague-Dawley rats were administered 0, 5, 50, 500, or 5,000 parts per million (ppm) di-n-octyl phthalate (DNOP) in their diet for 13 weeks. Similar control groups received either 4% corn oil or 5000 ppm of di(2-ethylhexyl) phthalate (DEHP). At termination, blood and tissue samples were obtained for selected analyses including specific liver enzymes, fat residue analysis, and peroxisome proliferation.

5. Toxicity

Id 117-84-0
Date 07.12.2006

Test substance : 1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate); CAS #117-84-0
Conclusion : Limited signs of toxicity were observed in male and female rats administered DNOP in the diet for 13 weeks.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
07.12.2006

(5)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Bacterial
Test concentration : 5 dose levels up to 10 mg/plate
Cytotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 1985
GLP : no data
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Method : A mutagenic response was defined as a reproducible, dose-related increase in the number of histidine-independent colonies over the spontaneous incidence. There was no requirement for a specific magnitude of increase.

Test condition : Approximately 10E8 bacteria were mixed with 0.5 ml of either 0.1M sodium phosphate buffer or S-9 mix, and test substance. The reaction was carried out in triplicate. The mixture was incubated at 37°C for 48 hours, after which time histidine-revertant colonies were counted. The doses selected were separated by half-log intervals. The high dose was 10 mg/plate unless limited by solubility. Positive control chemicals were sodium azide, nitro-o-phenylenediamine, 9-aminoacridine and 2-aminoanthracene. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest with TA100 was conducted to determine the high dose level.

Test substance : 1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate); CAS #117-84-0

Conclusion : No mutagenic activity was observed at doses up to 10 mg/plate in Salmonella strains TA98, TA100, TA1535 and TA1537 with or without metabolic activation.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
07.12.2006

(10)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type : Two generation study
Species : mouse
Sex : male/female
Strain : CD-1
Route of admin. : oral feed

5. Toxicity

Id 117-84-0

Date 07.12.2006

Exposure period	: Continuous throughout study (beginning 7 days prior to mating).
Frequency of treatm.	: Daily throughout premating, mating, gestation and lactation.
Premating exposure period	
Male	: 7 days
Female	: 7 days
Duration of test	: 2 generations
No. of generation studies	:
Doses	: 0.0, 1.25, 2.5, or 5.0% (0, 1.8, 3.6, and 7.5 g/kg/day)
Control group	: yes
NOAEL parental	: = 5 %
NOAEL F1 offspring	: = 5 %
NOAEL F2 offspring	: = 5 %
Method	: other
Year	: 1987
GLP	: no data
Test substance	: other TS: CAS #117-84-0; dioctyl phthalate
Method	: Cochran-Armitage (dose-related trends); Fisher's exact test (mating and fertility trends); Kruskal-Wallis test and Jonckheere's test (group means for sex ratio); Wilcoxon-Mann-Whitney U test (pairwise comparisons of treatment group means).
Remark	: DNOP had no effect on any fertility or reproductive measure. There were no treatment-related changes in parental clinical signs, body weight gains, or food consumption. The only significant finding was increased liver weight in the high dose (5%) males and females and increased kidney weight in the high dose females.
Test condition	: There were 40 animals/sex in the untreated control group. Males and females in the treatment groups (20 animals/sex) were exposed to the test substance beginning with a 7-day premating period and throughout a cohabitation period for approximately 14 weeks. Reproductive function was assessed during this cohabitation period for number of litters per pair, number of live pups, sex, live births, and pup weight. These litters were subsequently discarded. Following the 14-week cohabitation, the pairs were separated during which time any final litters were delivered and kept for assessment of the next generation fertility (F1). When the F1 litters were sexually mature, they were mated with animals from different litters within the same group. The F2 litters were examined for litter size, survival, sex and pup weight. The F1 animals were then sacrificed and necropsied. F0 parameters evaluated: clinical signs, mortality, body weight gain, consumption of food and water. F1 parameters evaluated: reproductive performance, litter size, survival, sex and pup weight F2 parameters evaluated: litter size, survival, sex and pup weight. Sperm examination: Epididymis from the right cauda was excised. The percentage of motile sperm, under 400 magnification was determined. Necropsies: In females, endpoints examined included organ weights and histology. In males, organ weights, histology, percentage of motile sperm, sperm concentration and percentage of abnormal sperm were assessed. Clinical observations were performed on blood and urine collected at the post-mortem examination.
Test substance	: 1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate); CAS #117-84-0
Reliability	: (1) valid without restriction
Flag	: Critical study for SIDS endpoint
07.12.2006	

(6)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	: mouse
Sex	: female
Strain	: CD-1

5. Toxicity

Id 117-84-0

Date 07.12.2006

Route of admin. : gavage
Exposure period : Gestation days 6-13
Frequency of treatm. : Daily
Duration of test : 7 Days
Doses : 10 ml/kg/day (9780 mg/kg/day)
Control group : yes
NOAEL maternal tox. : = 9780 mg/kg bw
NOAEL teratogen. : = 9780 - mg/kg bw
Method : other
Year : 1987
GLP : no data
Test substance : other TS: CAS #117-84-0; dioctyl phthalate

Result : NOAEL: 9780 mg/kg/day (maternal and developmental).

Maternal Effects: No mice died during the study. There were no clinical signs of toxicity or changes in food consumption or body weight.

Embryo/fetal Effects: The only differences from the concurrent control group were a slightly reduced number of live births per litter (10.2 vs. 11.5) and reduced pup weight gain (0.6 g vs. 0.7g). However it was noted that the control values for these parameters were significantly higher than other control values in this study program, therefore the differences were not considered to be biologically significant.

Test condition : Fifty timed-pregnant female mice were dosed daily on gestation days 6-13 with the test substance. A single dose level of 10 ml/kg was used as the highest practical level due to lack of toxicity (LD10 could not be established). Litters were held until postpartum day 3 then discarded. The following data were recorded: maternal observations, survival, and weight gain from gestation day 6 to postpartum day 3; number of live births, number of viable litters, total litter weight, litter weight gain, and pup survival.

Test substance : 1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate); CAS #117-84-0

Conclusion : No significant developmental effects were found at a single maximum dose level of 10 ml/kg/day (9780 mg/kg/day).

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

07.12.2006

(5)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY**10.2 HAZARD SUMMARY**

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physicochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

06.07.2006

10.3 RISK ASSESSMENT